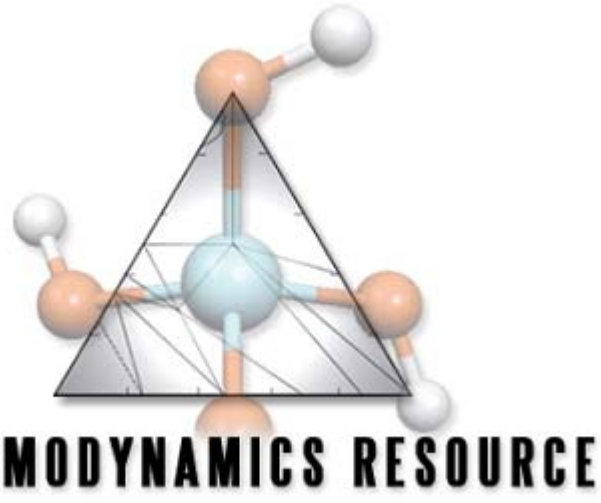
Industrial Technologies Program

Thermodynamics Resource: A User-Friendly Database of Thermochemical Information for High-Temperature Materials Processing and Corrosion

A Convenient Web-Based Tool Provides Access to Thermodynamic Properties Relevant to a Wide Range of Industrial Processes

Thermodynamic property data (heats of formation, heat capacities, and entropies for both condensed- and gas-phase compounds) are the foundation for building accurate models of all high-temperature processes. Such data has many applications, including: equilibrium calculations to predict corrosion of refractories and other materials; heat-transfer modeling of furnaces and molten phases of glasses and metals; modeling of high-temperature chemical reactions occurring in material synthesis; prediction of process energy efficiency and pollutant formation for combustion and other high-temperature manufacturing processes; and prediction of liquidus temperatures and the formation of crystalline inclusions in glass formulations. Without thermodynamic data, it would be difficult or impossible to even begin to model many high-temperature processes. The technology roadmaps developed by various industry groups, including glass, aluminum, and chemicals, describe many high-priority technology barriers and research needs that in some way require detailed knowledge of materials thermochemistry.



http://www.ca.sandia.gov/HiTempThermo/index.html

Benefits for Our Industry and Our Nation

- *12 TBtu saved from improved container and flat compositions for light-weight glass.*
- *23 TBtu saved in the glass industry due to new formulations for corrosion-resistant refractories for oxy/fuel glass melters.*
- *12.5% improvement in aluminum melting furnace energy utilization from new furnace designs utilizing more thermally stable refractories.*
- *Corrosion-resistant materials for the black-liquor gasifiers in the pulp and paper industry.*
- *Electricity savings through improved processes for the removal of impurities in secondary aluminum used in shape castings.*
- *Novel high-temperature, corrosion-resistant materials for the chemicals industry.*

Applications in Our Nation's Industry

This project has applications throughout industry:

- Agriculture
- Aluminum
- Chemicals
- Forest Products
- Glass
- Heat Treating
- Metalcasting
- Mining
- Petroleum
- Process Heating
- Steel

Project Description

The goal of this project is to provide thermochemical data and models for an important set of materials - refractories and glasses. Such data are the basis for determining the potential for chemical interactions among materials and are essential for predicting stability and corrosion. All data will be incorporated into a comprehensive web-based tool that will provide the necessary input for commercial application.

Barriers

- Very limited data for refractories, glasses, and high-temperature gas-phase species
- Absence of experimental data for model verification
- Lack of a consistent, documented, continuously updated, and fully open repository for data

Pathways

The objectives of this project will be achieved through (1) the creation of models and the development of theory needed to predict thermochemistry from first principles; (2) development of fundamental thermochemical data for critical systems; (3) teaming with NASA/Glenn Research Center to provide critical experimental data; and (4) creation of a user-friendly web site for distribution of project results.

Milestones

Results To Date

- Refined, highly accurate model for glass systems (Na-Ca-Al-B-Si-O) that agrees well with published phase diagrams
- More than 900 gas-phase compounds including species containing C, Al, Si, Cr, Mn, Fe, In, Sn, and Sb
- Web site that is open to the public with data available at no charge
- Convenient, user-friendly web-site format, including access to thermodynamic modeling tools

Future Milestones

- Provide data relevant to reduction of impurities in the aluminum industry, including the elements Mg, Ti, and Fe
- Develop a model for application to refractory corrosion in black liquor gasification in the pulp/paper industry, based on the model of the Na-Ca-Al-O system
- Compile web pages for individual Industries of the Future to provide thermodynamic data files specific to problems in each industry
- Provide data on oxychlorides for use in modeling processes in the chemicals industry
- Develop user interface to FactSage, a commercial thermodynamic code
- Expand data relevant to combustion processes, especially NO_x-related and halogenated hydrocarbons

Commercialization

A web site is now live and available to the public at: http://www.ca.sandia.gov/HiTempThermo/index.html which provides all the available data at no charge. The data is well documented with a clear pedigree, unlike most commercial (encrypted) databases. Since the site's launch on August 31, 2002, numerous upgrades have occurred, including: the addition of a recent news page; archived earlier versions of the data; an on-line equilibrium calculator; and an improved search engine. Users may now subscribe to the on-line user community.

Project Partners

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RHI Refractories
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Shell Oil Products Company, LLC
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A Strong Energy Portfolio for a Strong America

Energy efficiency and clean, renewable energy will mean a stronger economy, a cleaner environment, and greater energy independence for America. Working with a wide array of state, community, industry, and university partners, the U.S. Department of Energy's Office of Energy Efficiency and Renewable Energy invests in a diverse portfolio of energy technologies.

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